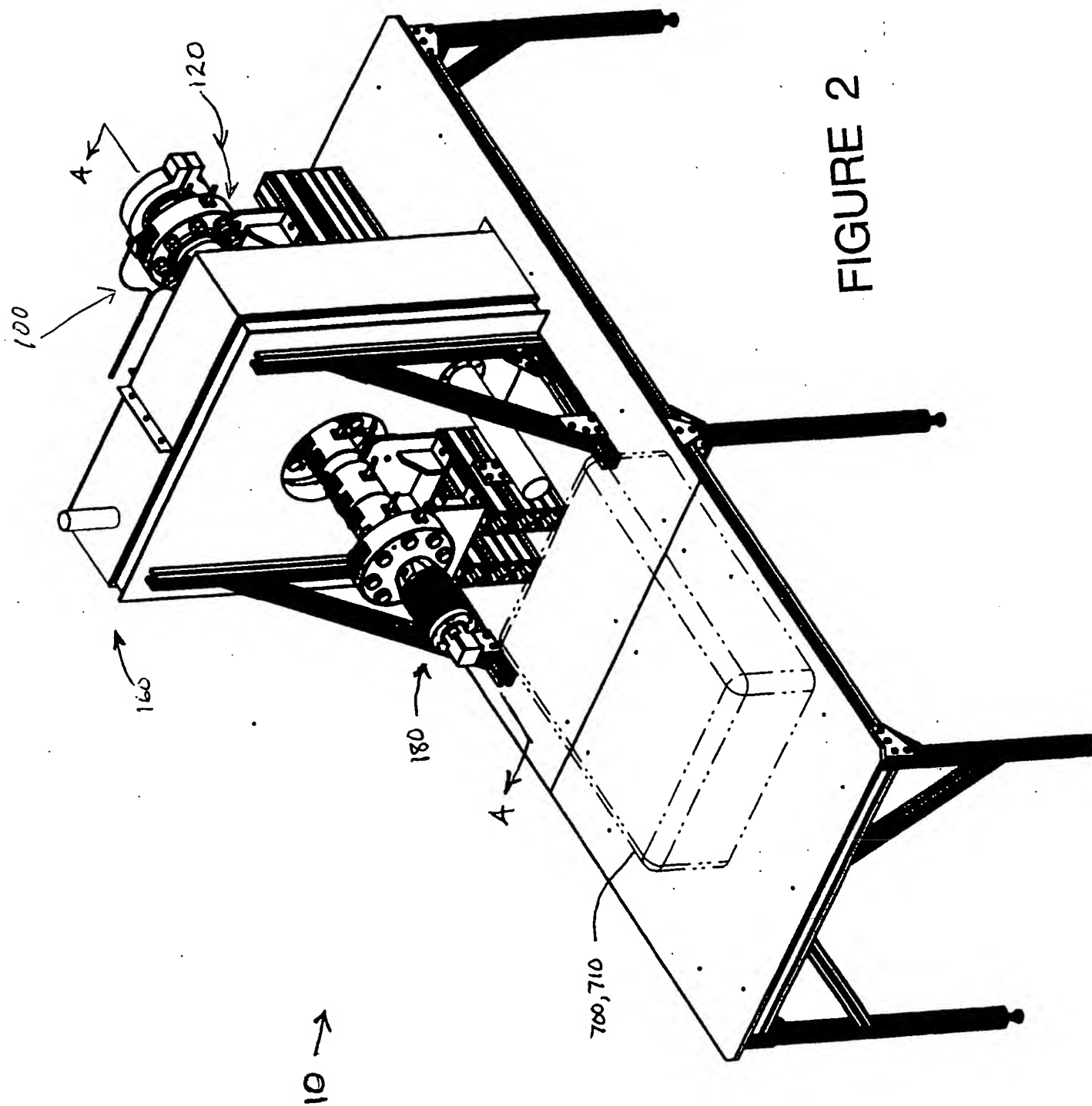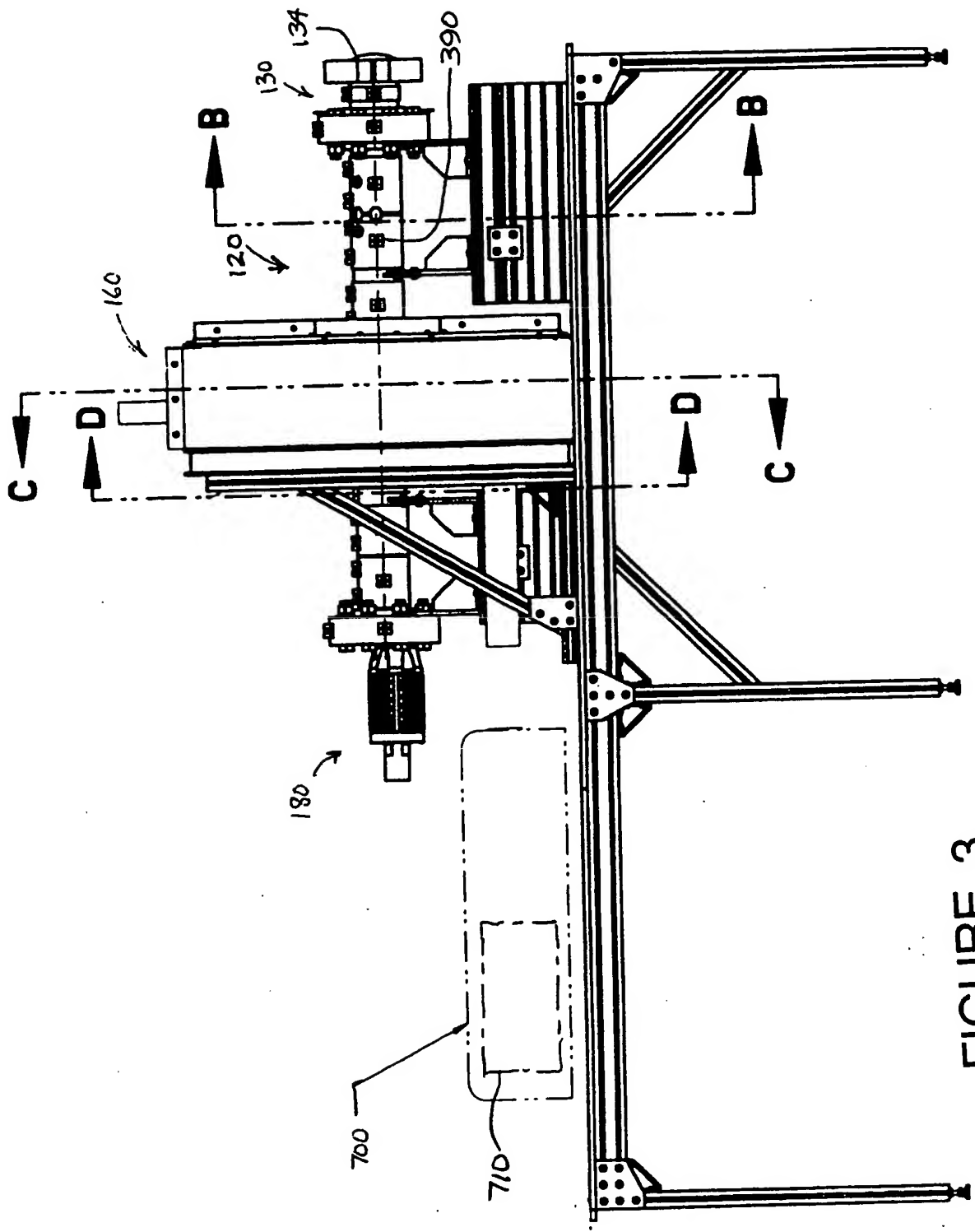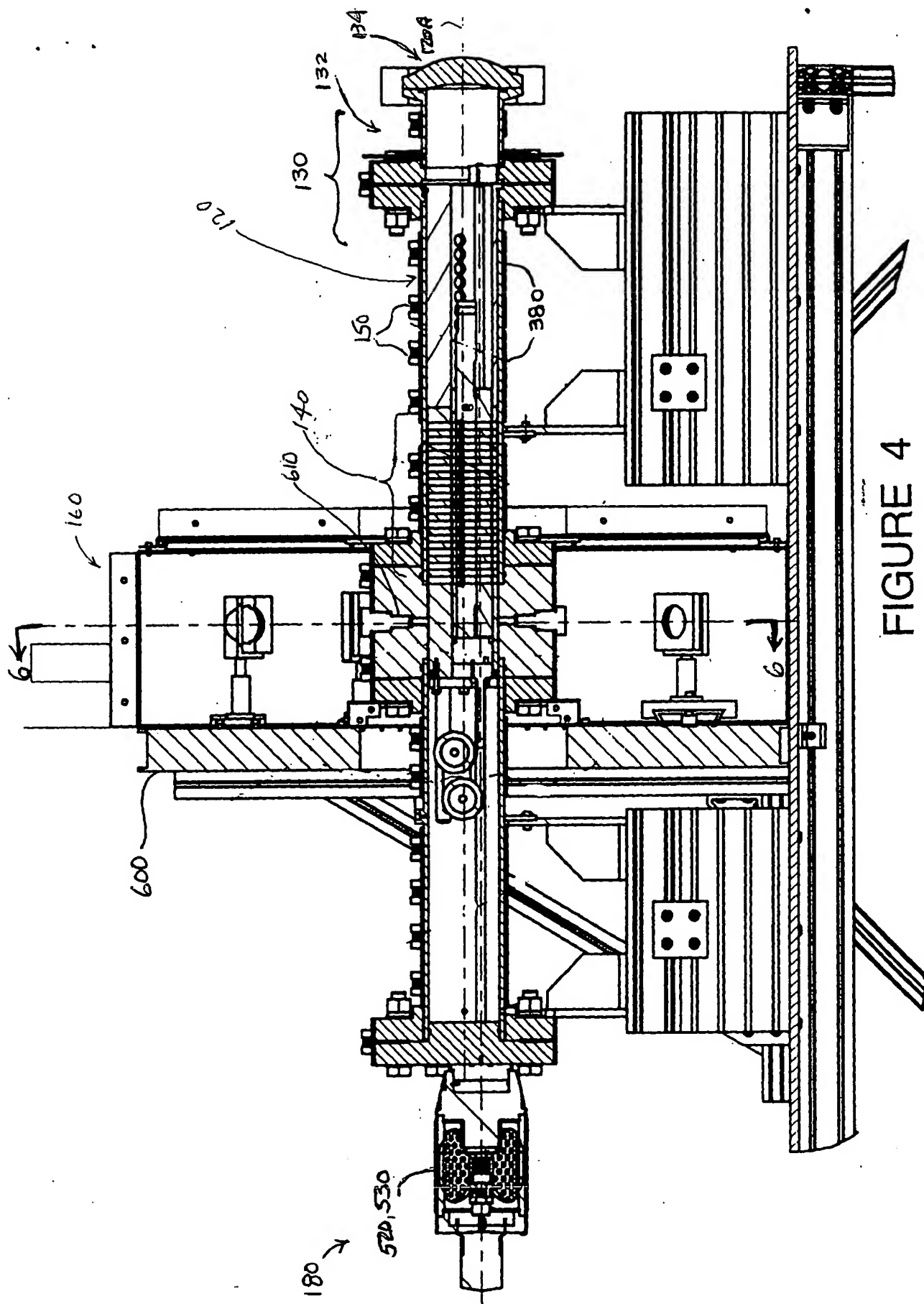FIGURE 1

FIGURE 2

FIGURE 3

FIGURE 4

FIGURE 5

FIGURE 6

500

340

320

300

390

392

FIGURE 7

FIGURE 8

362 908

120

500

810

VIEWING GAS
FLOWING "IN"

450

TO DETECTOR

642

FROM
LIGHT SOURCE
L

360

906

504

320

S

400

FIGURE 10

906

500

320

360

120

362

810
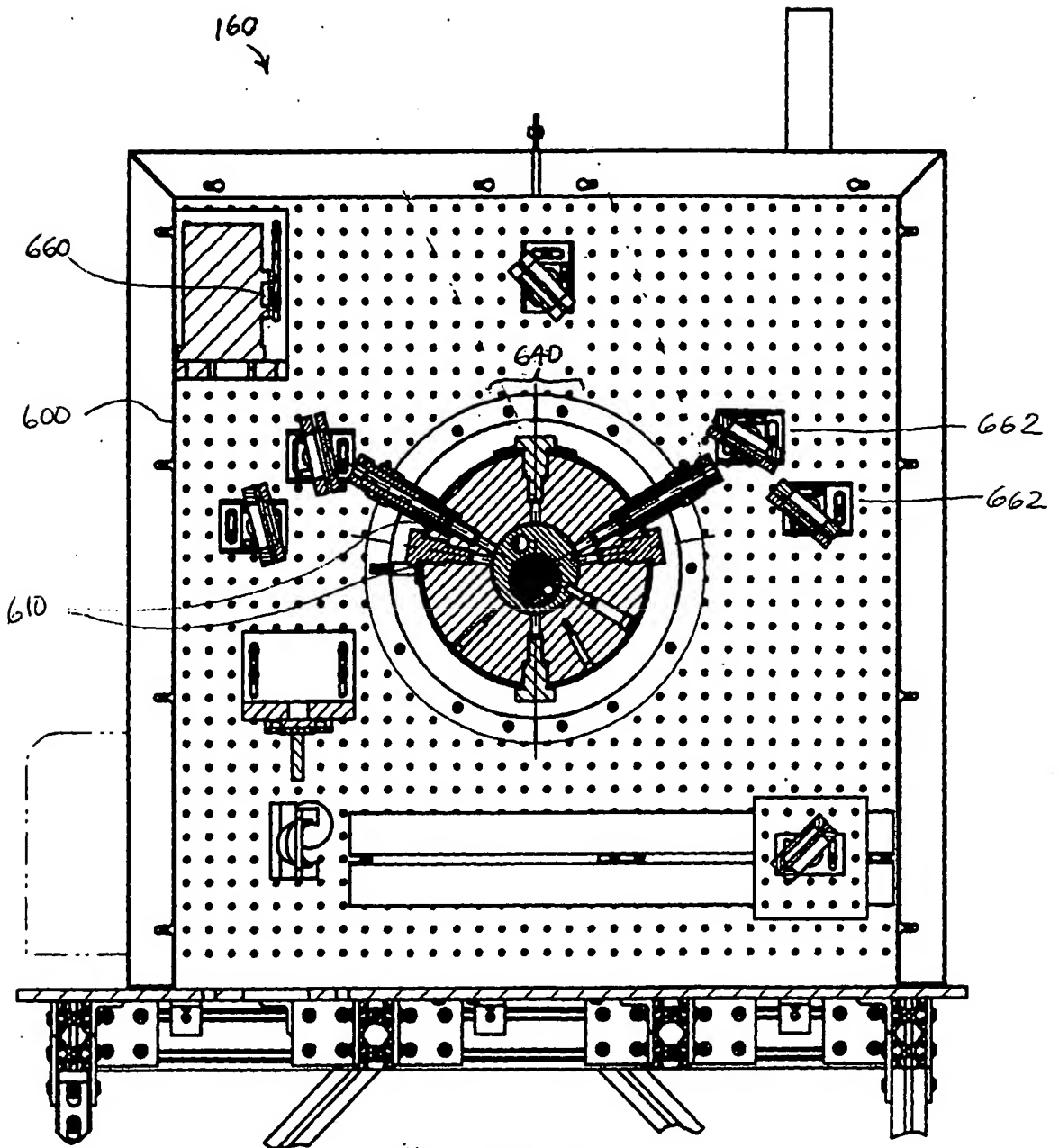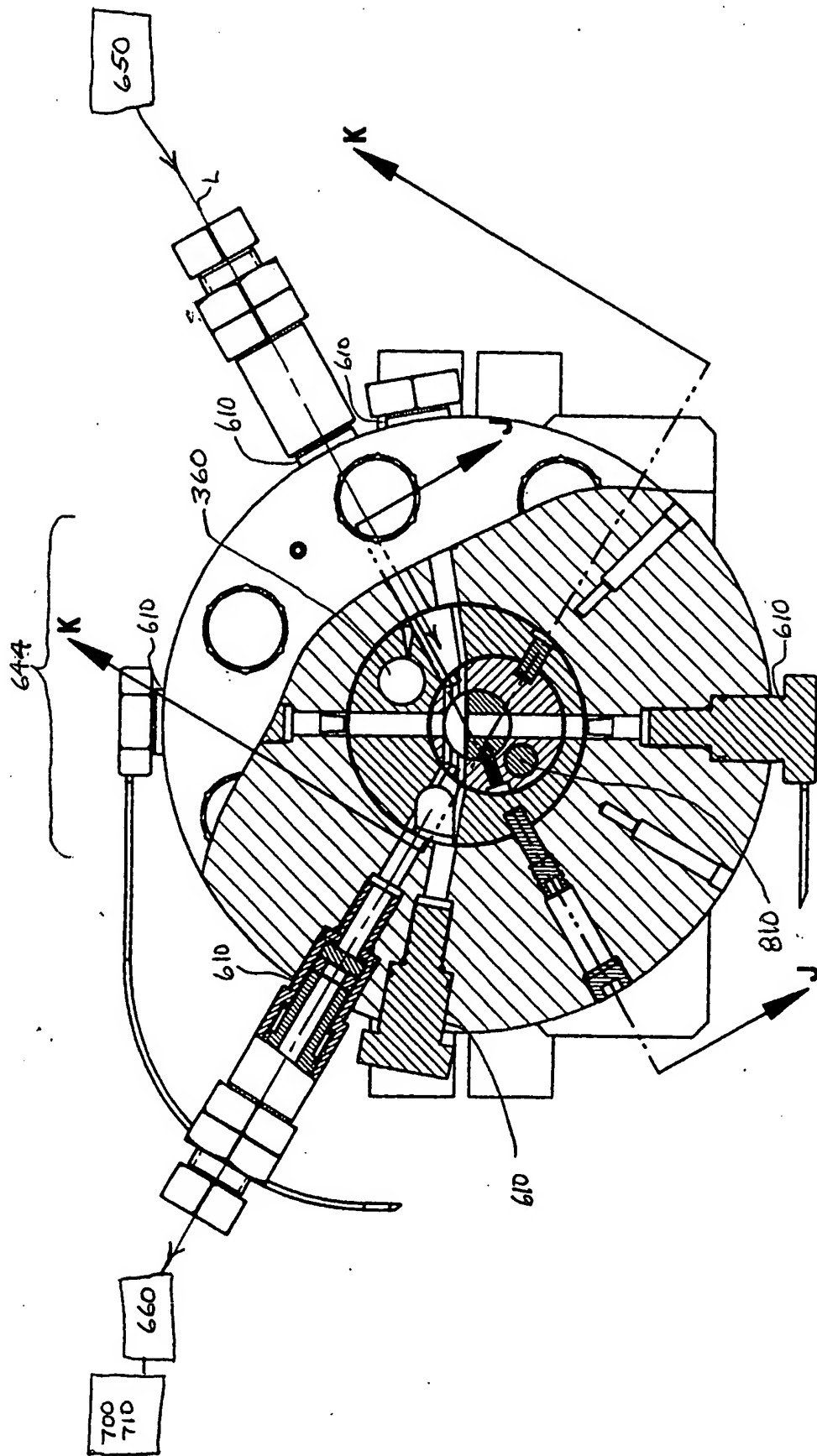
VIEWING GAS
FLOWING "OUT"

450

400

908
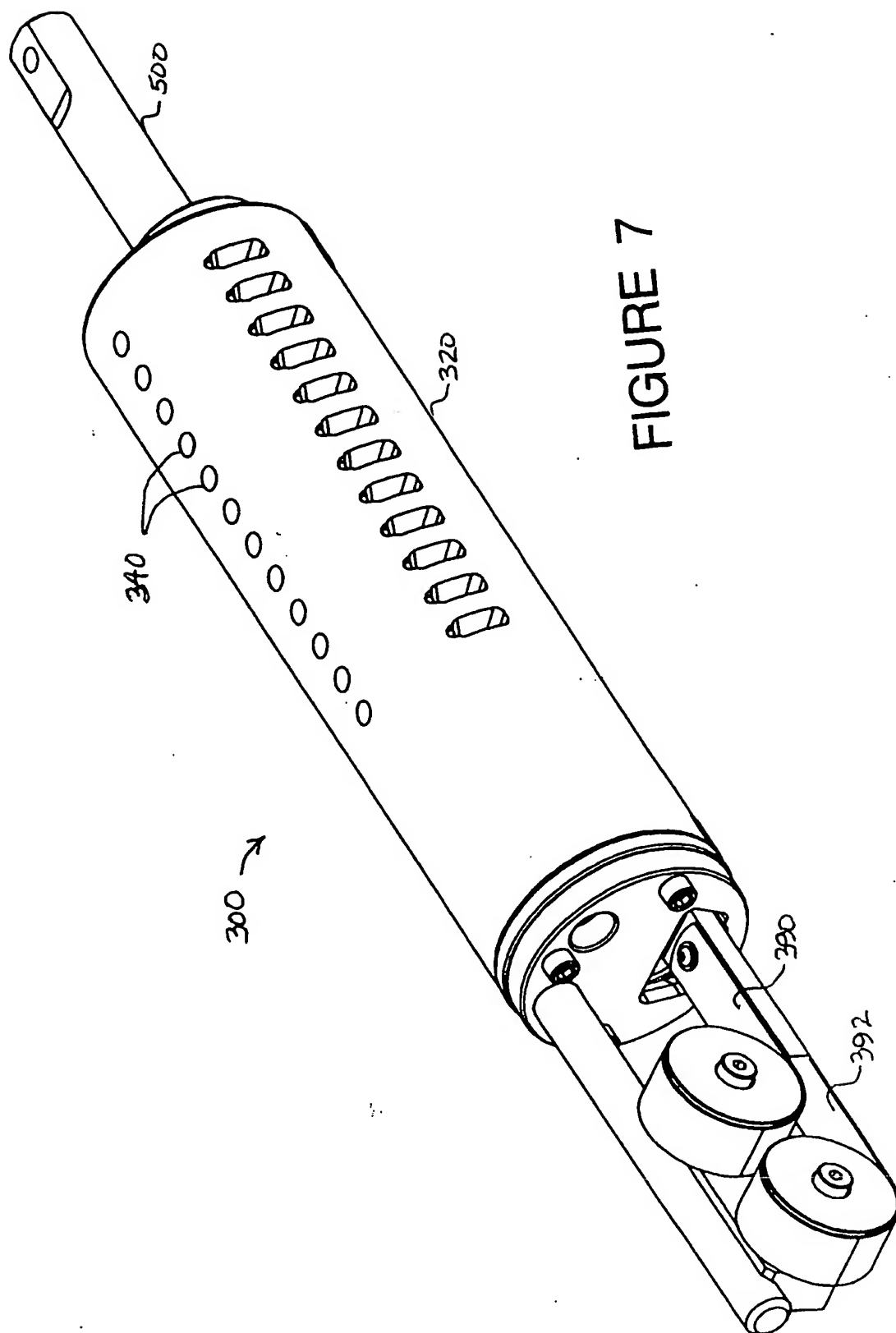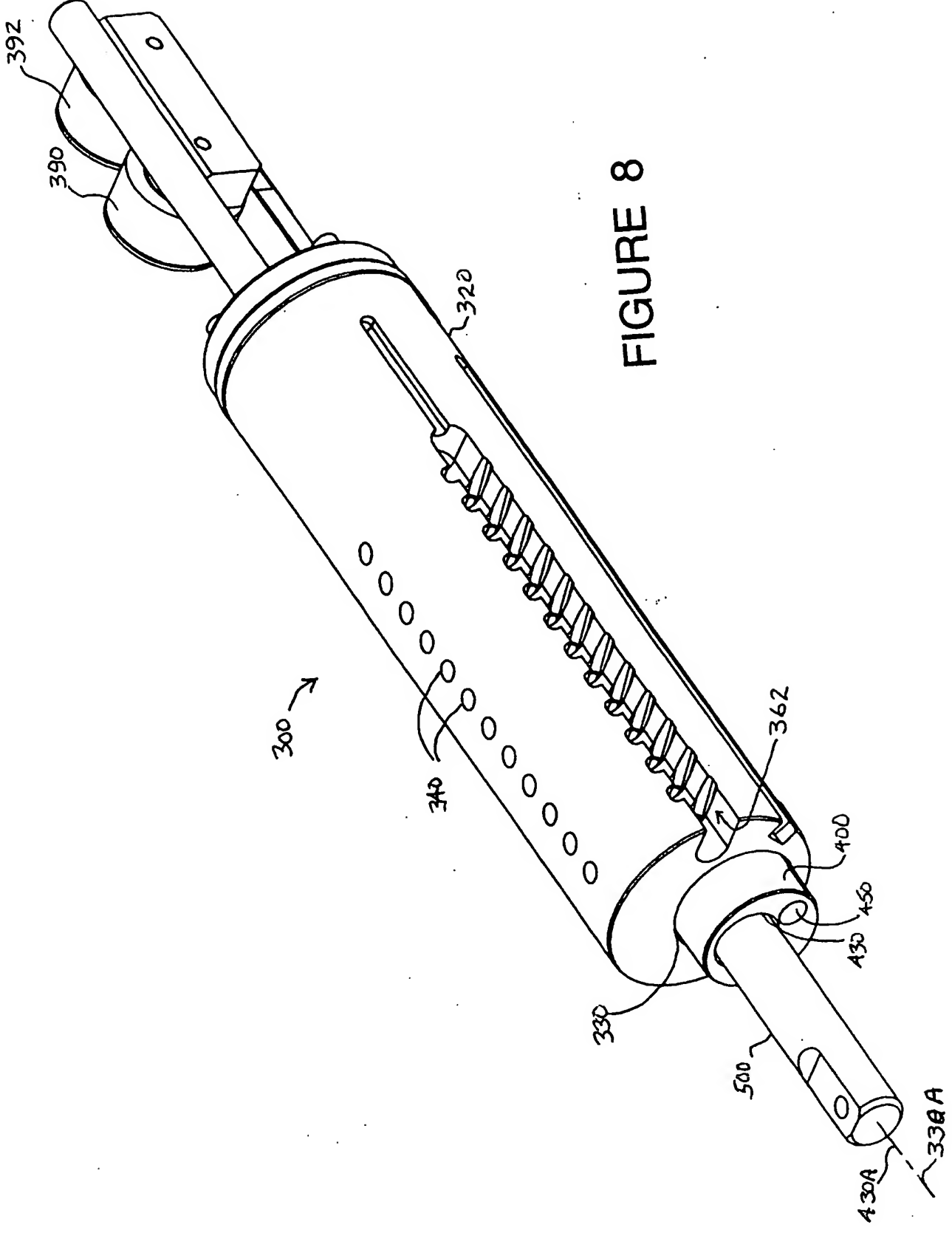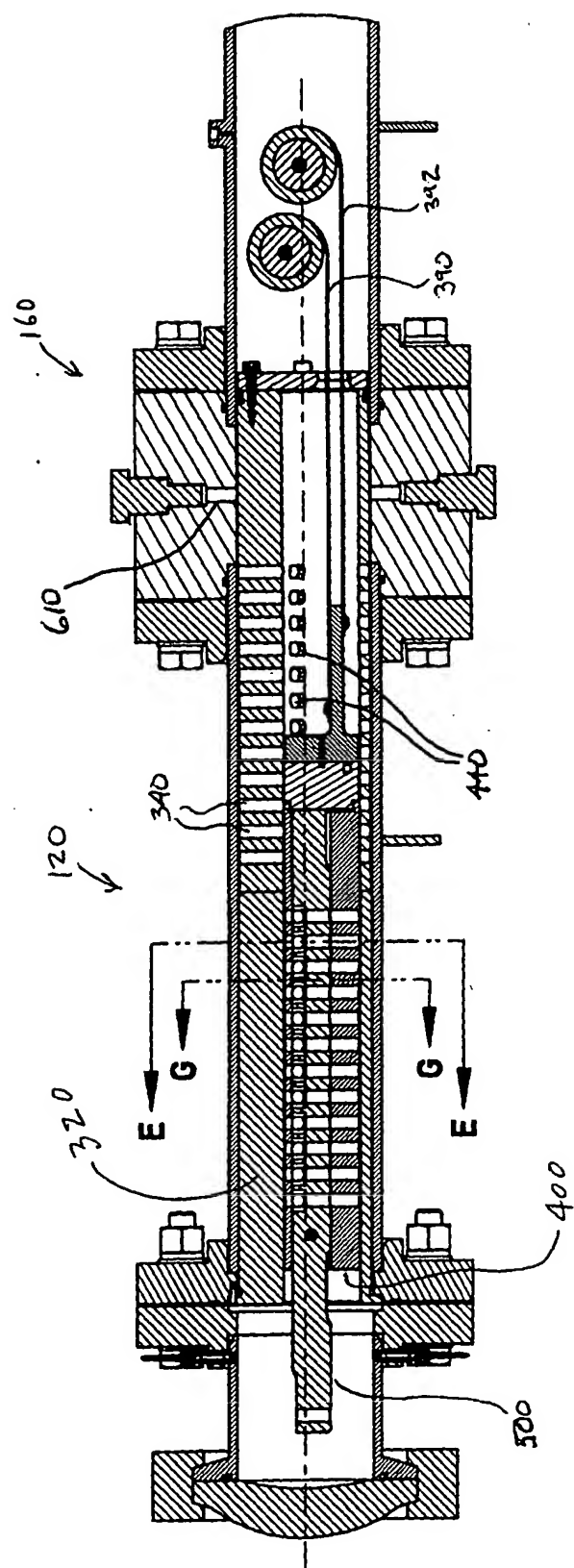
FIGURE 9
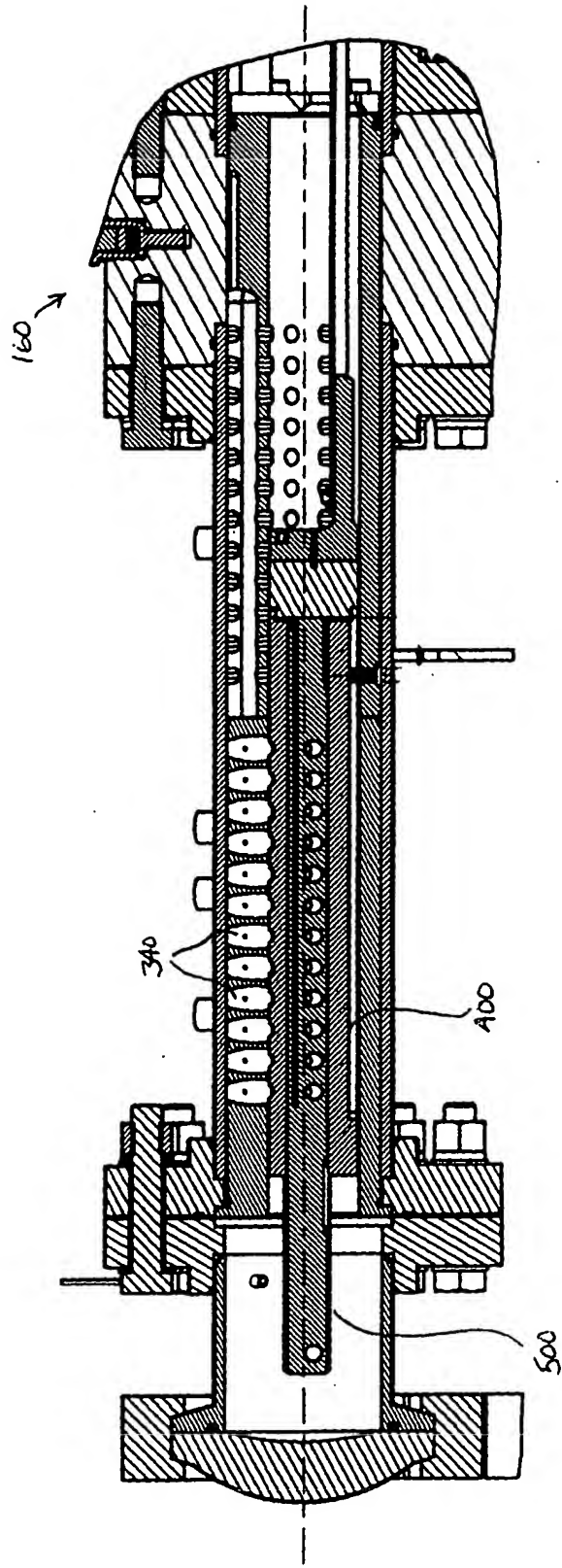
FIGURE 11

FIGURE 12
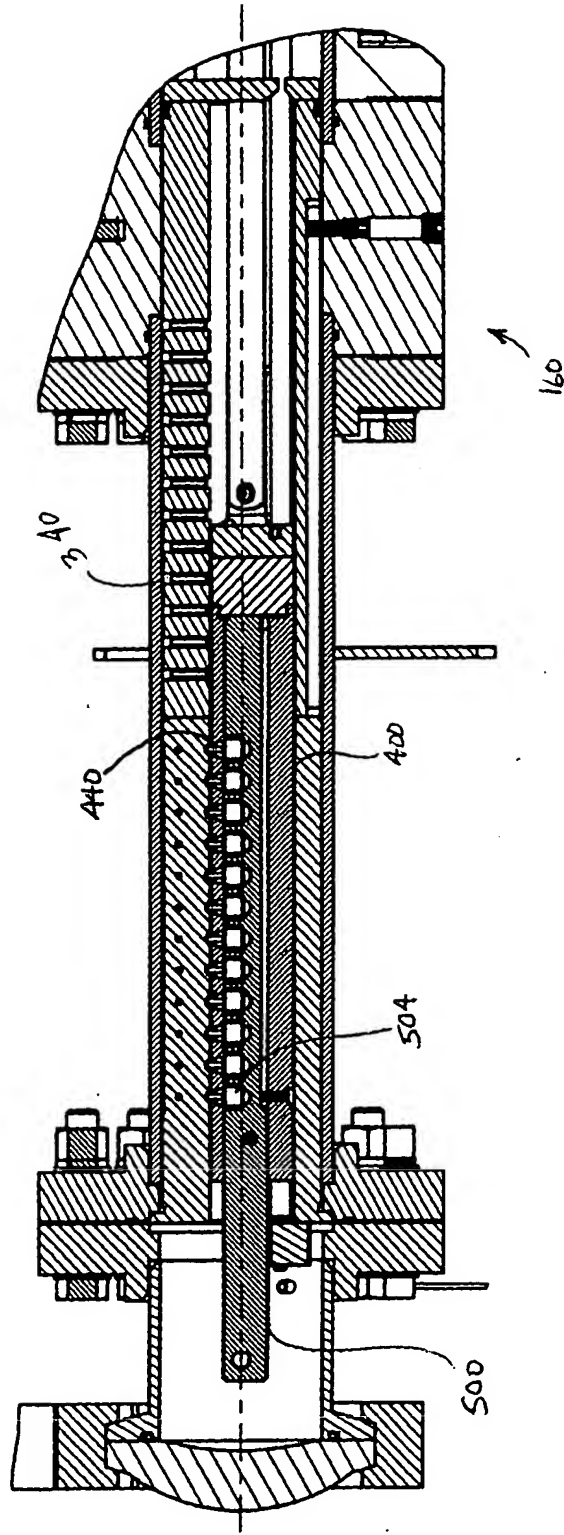
FIGURE 13

FIGURE 14

FIGURE 15

500

520

530

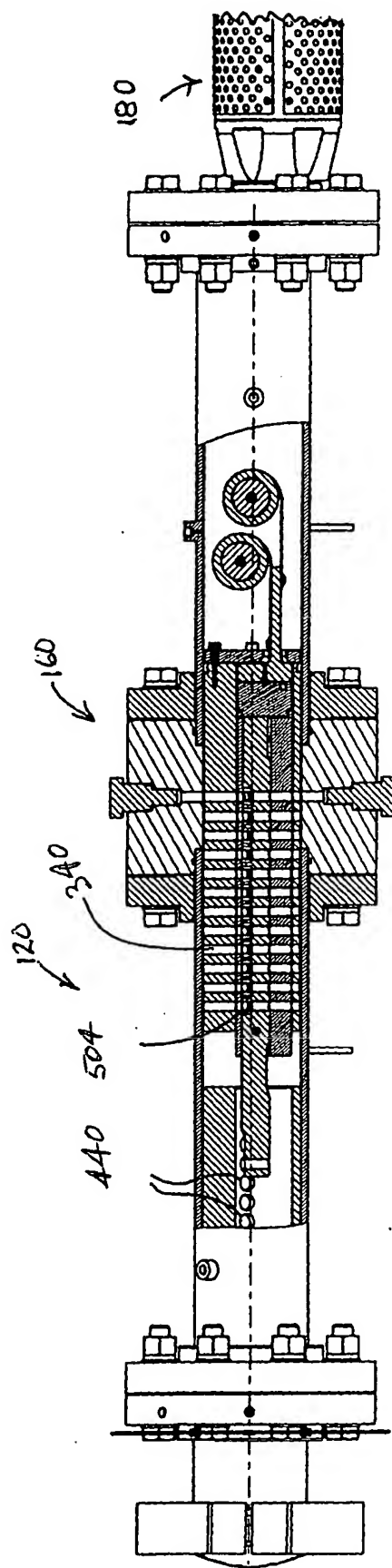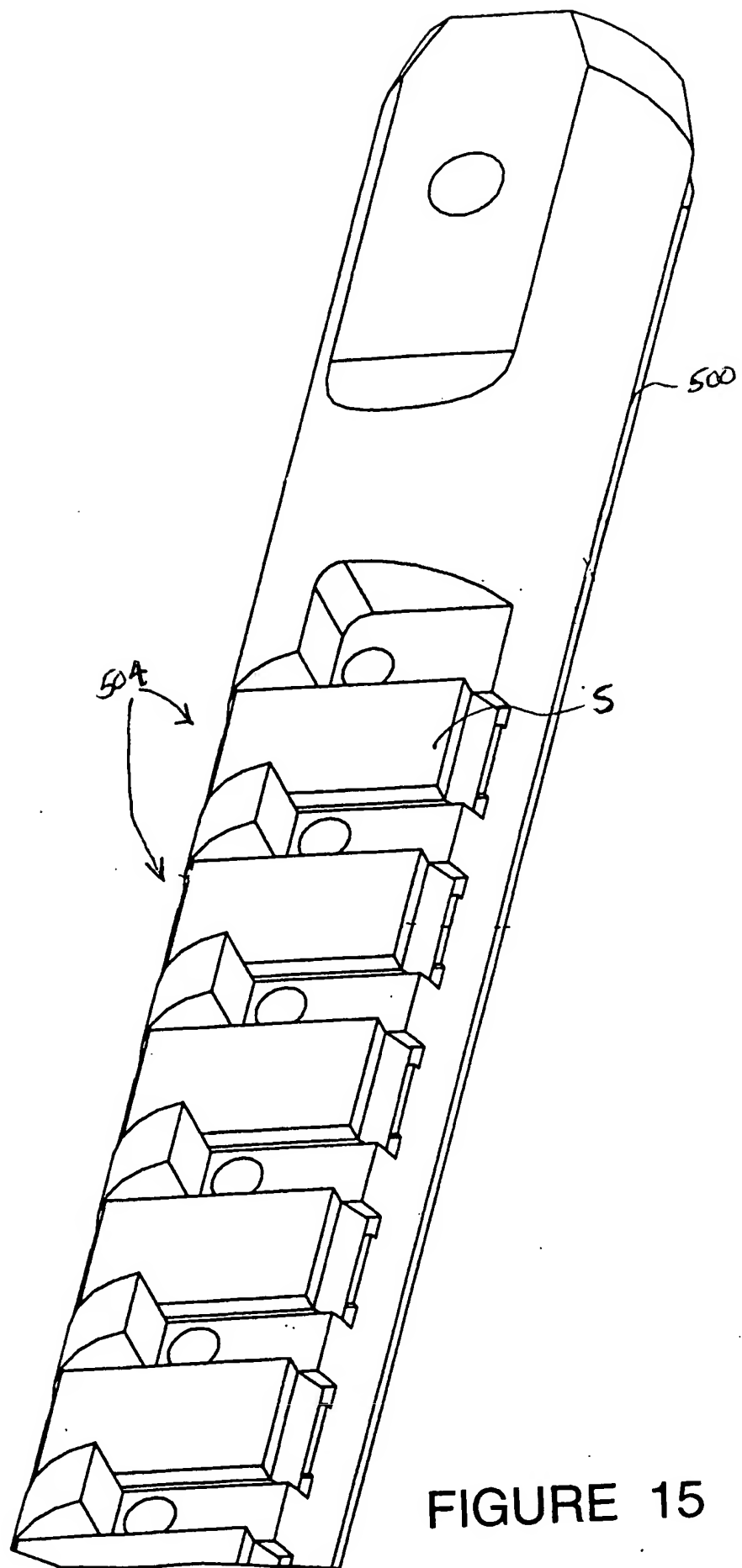504   506
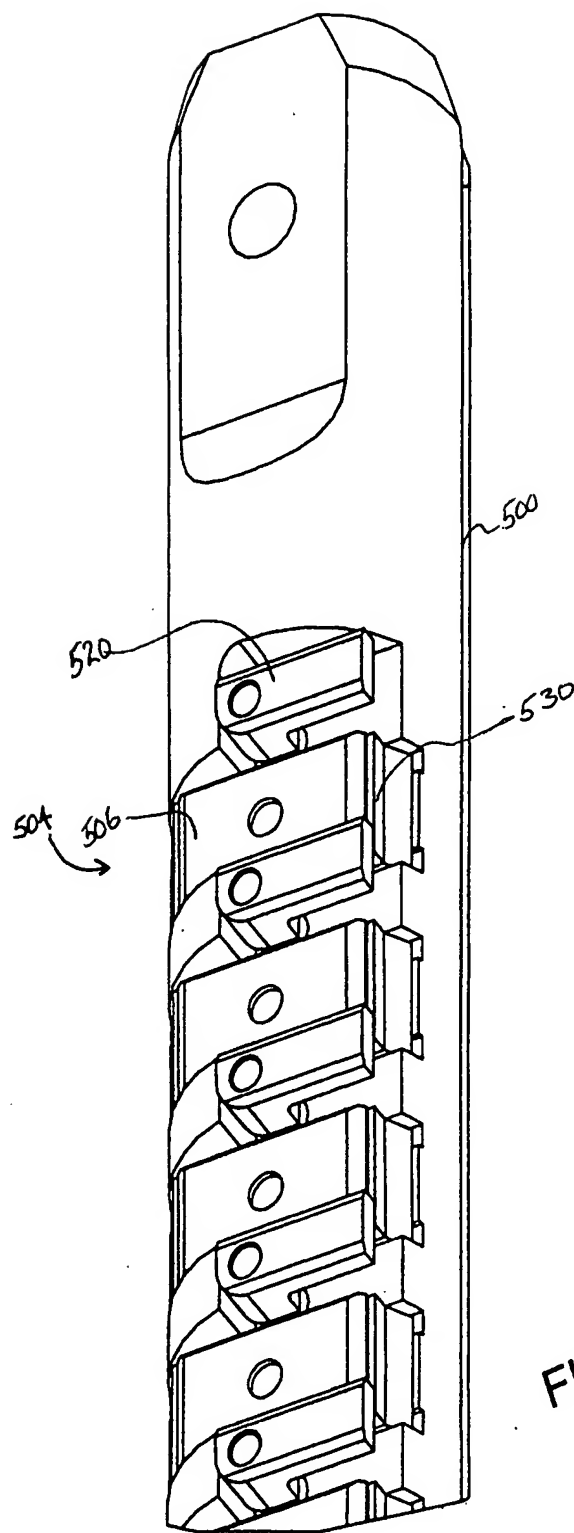
FIGURE 16A

CLAMP "UP" IN RELEASE
POSITION
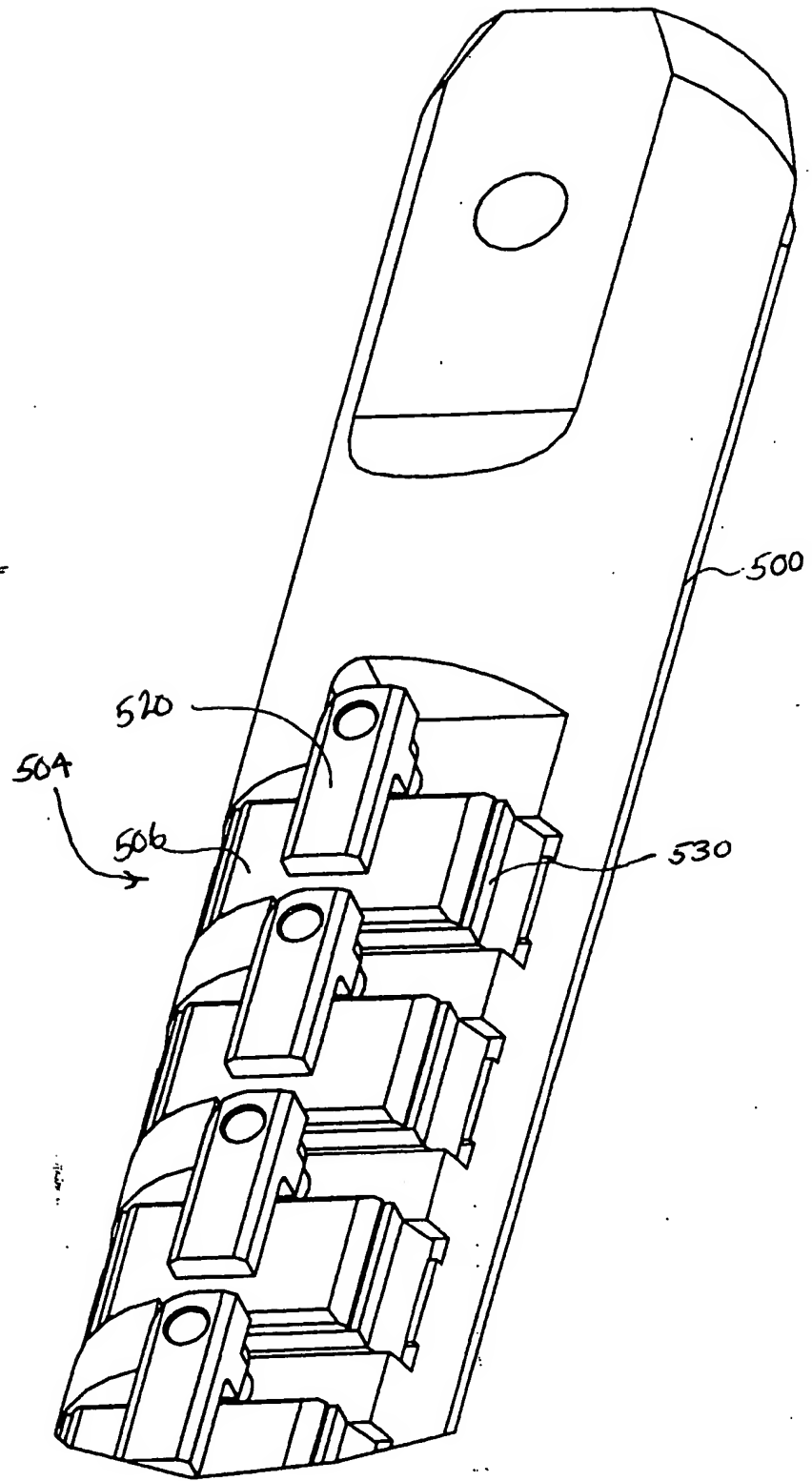
FIGURE 16B

CLAMP "UP" IN HOLDING
POSITION
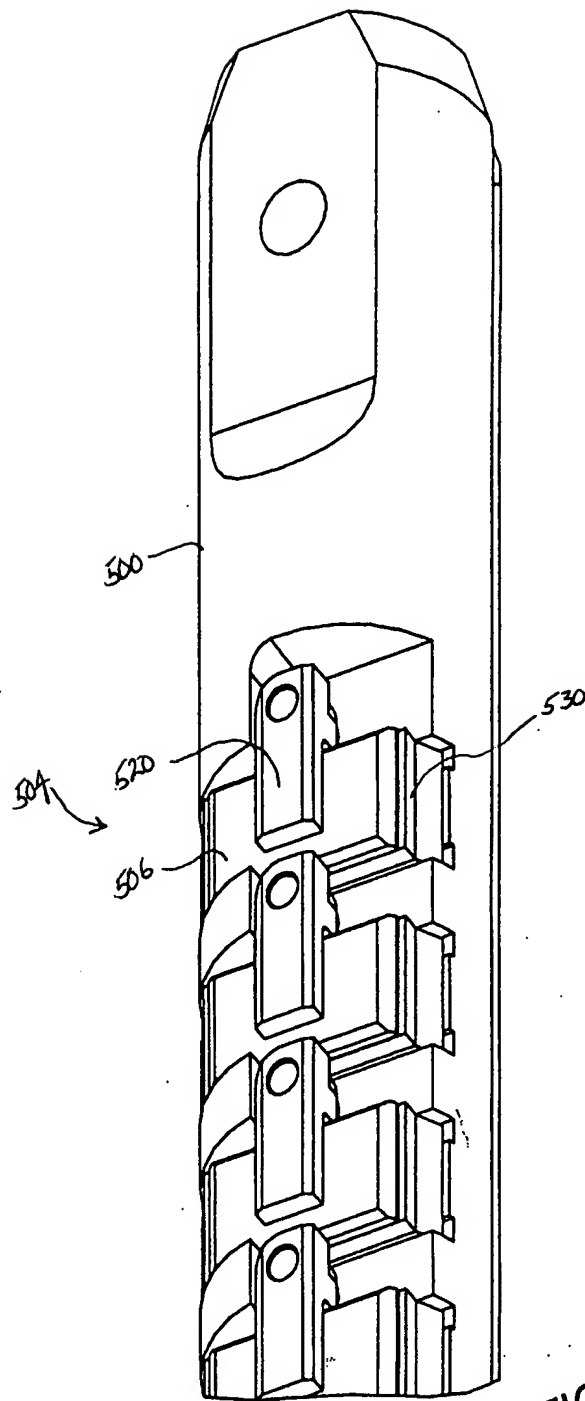
500

504

520

530

506

FIGURE 16C

CLAMP 'DOWN' IN HOLDING
POSITION

FIGURE 17

500

530

520

506

508

(.080) [2MM] MAX
SAMPLE THICKNESS SHOWN.
(0.020) [0.5MM] MIN
SAMPLE THICKNESS

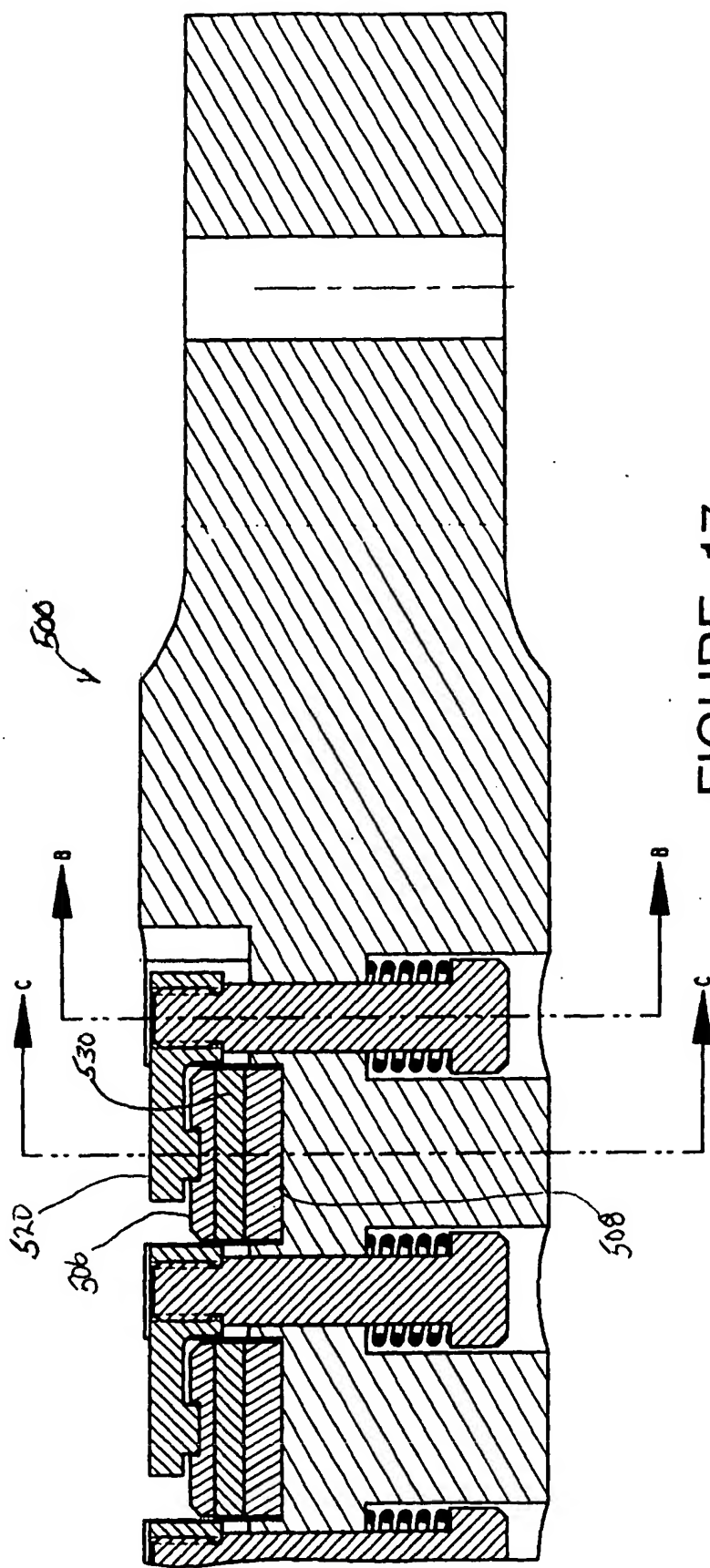(.030)

620

506

530

508
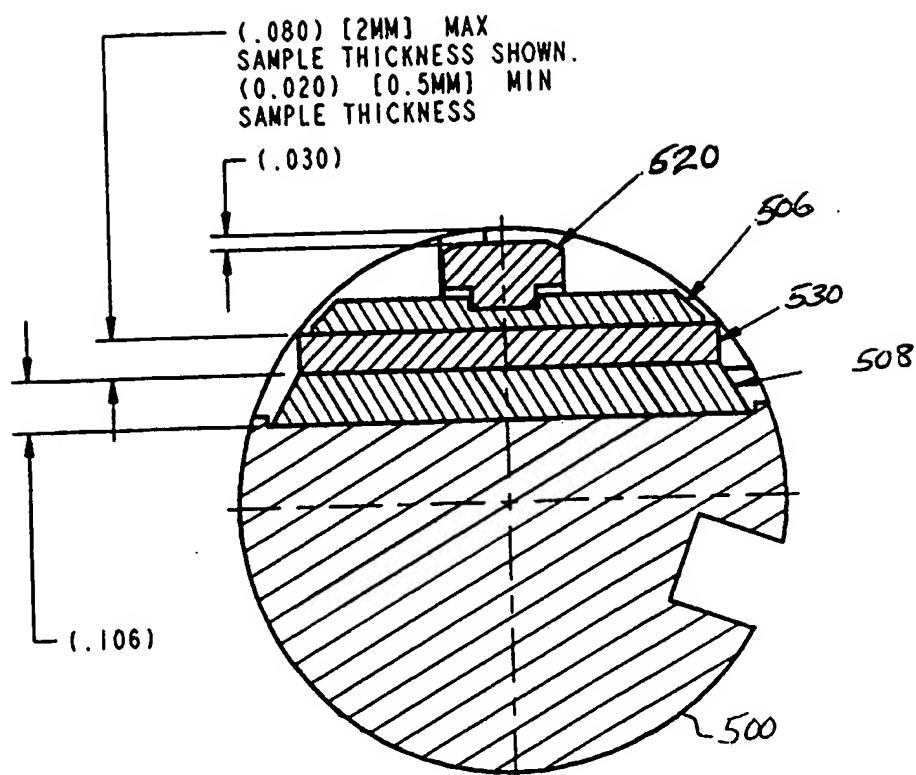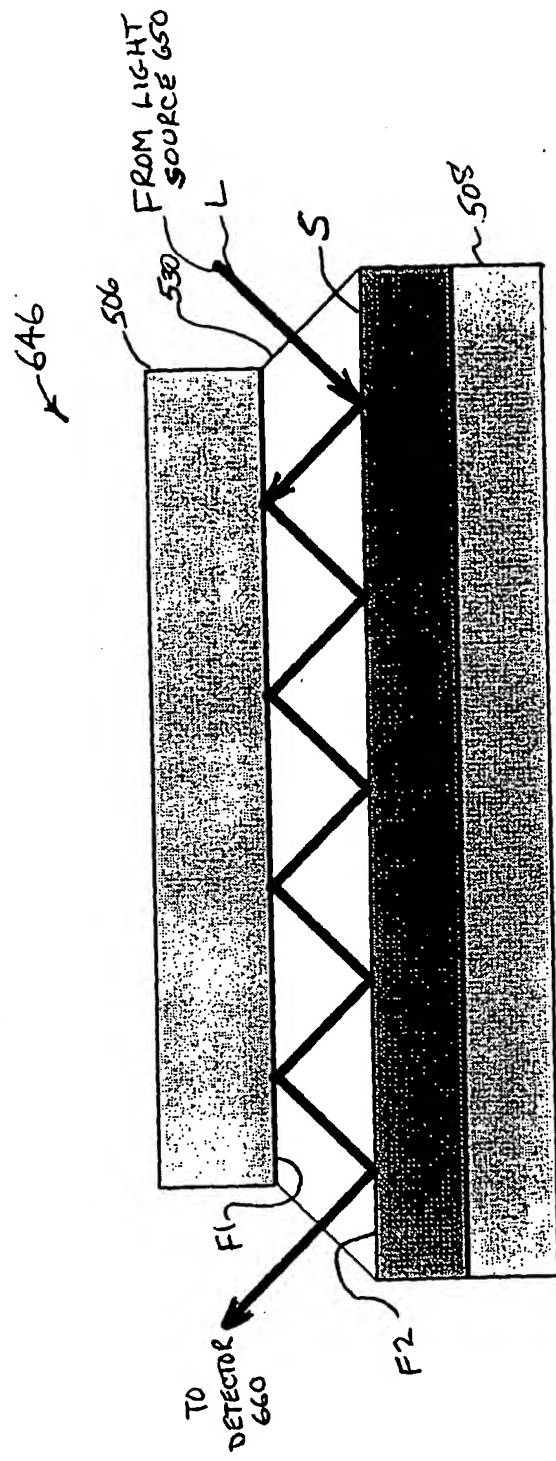
500

(.106)

FIGURE 18

FIGURE 18A

Button SetUp
    Button SetPoints
        Form SetPoints
            Function Activate Omegas

> Initiates software communication link between this application and the temperature controllers for the reactor and process.

            Function Save Set Points

> The user enters the temperature set point, maximum safety limit temperature and check box to activate each temperature zone in the reactor or process.
>
> This function then stores these settings as the new defaults as well as in records describing the experiment.

            Function Send Set Points

> Sends the temperature set points, safety limits and enable flag data to the temperature controller.

            Function Dismiss

> Removes this form window from the computer screen.

Button DataPath
    Form DataPath
        Function Make Directory

> Creates a new directory to store data files and records associated with an experiment.

        Function Apply

> Sets the storage directory for data files as the path selected in the displayed directory box.

        Function Dismiss

> Removes this form window from the computer screen.

Button Motor
    Form Motor
        Function Go

> Directs the motor to send the sample position to the optical measurement position

        Function Go To Load Position

> Directs the motor to send the sample canoe to the load position.

        Function Record Settings

> Stores in memory which sample positions will be observed/skipped during an experimental run loop.

        Function Update Status

> Updates the displayed status attributes of the motor, such as permission to move, current position, limit indicators, position error, motor overheating and motor power.

        Function Stop Motor Now

> Sends an immediate message to the positioning motor to stop moving.

        Function Dismiss

> Removes this form window from the computer screen.

    Button Calibrate Motor
        Form Calibrate Motor
            Function Update Status

> Updates the displayed status attributes of the motor, such as current location, home limit indicator, permission to move and position error.

            Function Go

> Directs the motor to send the selected sample position to the optical measurement position.

            Function Set Sample Location @ Current

> Stores in memory the current absolute motor position as the location at which the selected sample position is in the optical measurement position.

            Function Nudge the Motor

> Directs the motor to move the sample canoe in the relative direction and distance indicated by the slider.

            Function Stop Motor Now

> Sends an immediate message to the positioning motor to stop moving.

            Function Go There

> Directs the motor to move the sample canoe to the absolute position entered in the text box.

            Function Find Diode

> Directs the motor to move the sample canoe toward the reactor opening and stop when it reaches the home diode indicator.

Figure 19

            Function Find Load Position

> Same as Find Diode, but also travels to the load position, where the samples are positioned in the load/unloading gas manifold.

            Function Record All Parameters and Reset Motor

> Stores all motor control parameters and positions in a permanent configuration file and sends these parameters to the motor memory.

            Function Read Control Parameters

> Reads the current motor control parameters in the motor memory. Displays these values in a new pop-up window.

            Function Dismiss

> Removes this form window from the computer screen.

Button OceanOptics

    Form OceanOptics

        Function Correct Dark

Activates internal circuitry in the UV/Vis spectrometer to correct for purely-electronic, dark signal error.

        Function View Test

Collects an immediate UV/Vis spectrum and displays the spectrum in a pop-up window.

        Function Apply Settings

Stores UV/Vis spectrometer settings entered in the form to the spectrometer hardware, computer memory and configuration files.

        Function Dismiss

Removes this form window from the computer screen.

Button Nicolet

    Form Nicolet

        Function Bench Set Up

Activates FTIR spectrometer software to configure the FTIR processor, optical assembly and associated hardware.

        Function Invoke OMNIC

Activates vendor FTIR software for data visualization and processing.

        Function Apply Settings

Figure 20

Stores all FTIR spectrometer settings entered in the form to the spectrometer hardware, computer memory and configuration files.

        Function Dismiss

Removes this form window from the computer screen.

Button Parameters

    Form Parameters

        Button Set Path

            Form Data Path

        Function Write Experiment File

Records all parameters and setttings in a configuration file which would be required to describe and reproduce exactly the current experiment.

        Button Read Settings Experiment File

Opens the Read Setting Experiment File form

        Form Read Settings Experiment File

            Function Read

Restores a complete set of parameters and settings from the previously written experiment file displayed in the file directory box.

            Function Read + Set Path

Same as Function Read, but also sets the directory to store new data as the same directory as the experiment file to be selected and read.

            Function Dismiss

Removes this form window from the computer screen.

        Button Set Motor Positions

            Form Motor

        Function Refresh

Figure 21

Updates the listing of all experimental setting and parameter values listed in the text area in the upper right section of this form.

        Function Dismiss

Removes this form window from the computer screen.

Button Configuration
>**Form Configuration**
>>**Function Record These Ports**

Permits the user to assign computer serial port numbers to the interfaced instrumentation, such as the motor, UV/Vis spectrometer, temperature controllers and analog/digital signal converter.

>>**Function Record These Names**

Permits the user to assign zone names to pressure and temperature sensing signals.

>>**Function Check Installation**

Figure 22

Runs a test to ensure the software and its requisite resources are installed, configured and working properly.

>>**Function Dismiss**

Removes this form window from the computer screen.

Button Process
>**Button Open/Close Valves**
>>**Form Open/Close Valves**
>>>**Function Send**

Transmits signals to the solenoids to either open or close the Load In and Load Out valves, depending on the radio button selections on the form.

>>**Function Dismiss**

Removes this form window from the computer screen.

>**Button Set Points**
>>**Form SetPoints**
>**Button Show Process**
>>**Form Show Process**
>>>**Function Update**

Figure 23

Displays the current temperature and pressure zone names and attributes, such as control set point, current value, maximum limit, enable status and heating power output.

>>**Function Dismiss**

Removes this form window from the computer screen.

>**Function Auto-Tune Omegas(!)**

Initiates the temperature controller firmware which begins heating the process zones while computing optimal PID controller parameters.

>**Function Show Process Logs**

Displays a pop-up window which displays the recent history of process temperatures, process pressures, system messages and experimental events.

Button Experiment
    Button Parameters
        Form Parameters
    Button Apply
        Function Apply

Updates and records all parameters and settlings in memory which would be required to describe and reproduce exactly the current experiment.

    Button RUN !!
        Function RUN

Activates the automated run sequence for an experiment. The run sequence is displayed in the Parameters form.

    Button Pause
        Function Pause

Pauses the automated run sequence or Resumes the current run sequence.

Button Data
    Button View IR Spectrum
        Function View IR Spectrum

Activates vendor software to display and analyze a recorded FTIR spectrum.

    Button Analyze IR Series
        Form Analyze IR Series
            Function Select

Use the data in the file currently selected in the file list box as a background reference to compute new peak heights and areas.

            Function View

Display the data in the file currently selected in the file list box as a spectrum with the previously selected background reference. The user may select regions to define the appropriate baseline and peak integration limits.

            Function Apply

Record and use the previously selected baseline and peak integration limit

            Function Process

For the data in each file over the range of files selected in the form, integrate the absorbance peak using the background, baseline and limit specifications displayed in the form. Write the collection time and peak area data in a result file.

Figure 24

            Function View Data

Invoke a Notepad editor to view the aforementioned result file.

            Function Dismiss

Removes this form window from the computer screen.

    Button Export IR Series
        Form Export IR Series
            Function Make Dir

Create a new directory in which to store the new data files which will be generated.

            Function Run

Convert the data in the selected file sequence from their current data format into the format selected in the list box. Store each data file set in a new file with the same file name and new format suffix.

            Function Dismiss

Removes this form window from the computer screen.

Button View UV/Vis Spectrum
    Function Invoke UV/Vis

Begin the execution of a program to view UV/Vis spectra recorded during a previous experiment.

Button Analyze UV/Vis Series
    Function Invoke UV/Vis

Begin the execution of a program to analyze UV/Vis spectra and absorptions recorded during a previous experiment.

Button Export UV/Vis Series
    Function Invoke UV/Vis

Begin the execution of a program to convert data in one format to another.

Figure 25

Button Set Motor's Home Position
    Form Set Motor's Home Position
        Button Sample Boat Is Installed
            Function Sample Boat Is Installed

motor is safe to operate. The function begins a sequence to find the sample canoe standard load position. If the sequence is successful, permission is granted to move the motor.

        Button Cancel
            Function Cancel

The user selects this button when he cannot confirm that the sample boat is properly loaded. The software does not set the home position and does not grant permission to move the motor.

Button Emergency Motor Stop
    Function Emergency Motor Stop

The motor is sent an immediate message to stop motion, the experiment is terminated and the program is terminated.

Button Exit and Kill
    Form Exit and Kill
        Function Exit

The user confirms that he wishes to terminate the program.

        Function Cancel

Removes this form window from the computer screen.

Key:

The software follows the familiar windows, event-driven mode of operation. The software does nothing until the user presses a button. The button pressing event may alter the viewable buttons or activate Forms and Functions. Forms and Functions are encoded as software subroutines. The various buttons and functions are identified by the label observed by the user on the forms

    Form

A form presents a window on the user's computer screen. This form may present information, controls, input objects (such as text boxes, radio buttons, menus, lists, sliders), pictures, and command buttons.

    Button

A button (or command button) is pressed to execute a software command. The button typically begins the execution of a function, but may also expose new forms or replace the current set of viewable buttons.

    Function

A function initiates the execution of a software module which is typically a Visual Basic subroutine or function.

Figure 26